Project Overview

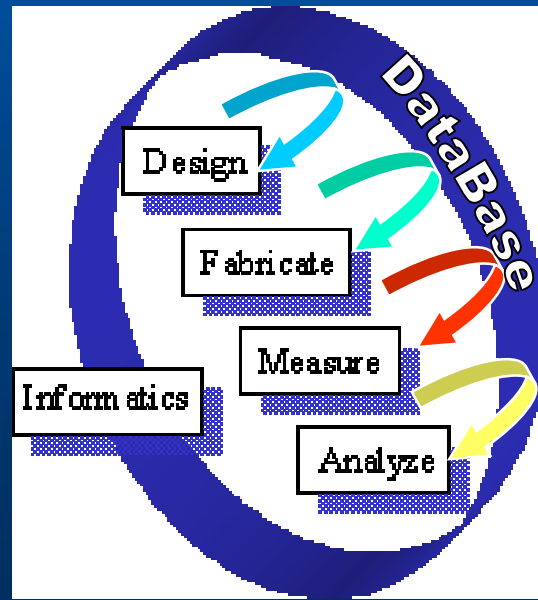
Combi Informatics System

Polymer Division: Wenhua Zhang, Mike Fasolka, Amit Sehgal
Alamgir Karim and Eric J. Amis
CTCMS: Andy Roosen, James Warren

Project Goal – Closing the Loop

Informatics & feedback for:

- **Data management, integration**
- **Automated data entry, retrieval**
- **Protocols to standardize data formats**
- **Link to and refine other Combi processes**
- **Library of scientific combi-data**
- **Data visualization**



Progress

- Database system selection
- Database server setup
- Security / data protection issues
- Basic framework of the database
- Backbone interface programming
- Instrument programming

PostgreSQL

- **Sophisticated Object-Relational DBMS**
- **Supporting almost all SQL (Structured Query Language), including subselects, transactions, and user-defined types and functions**
- **One of the most advanced open-source database available anywhere**
- **Commercial support available**

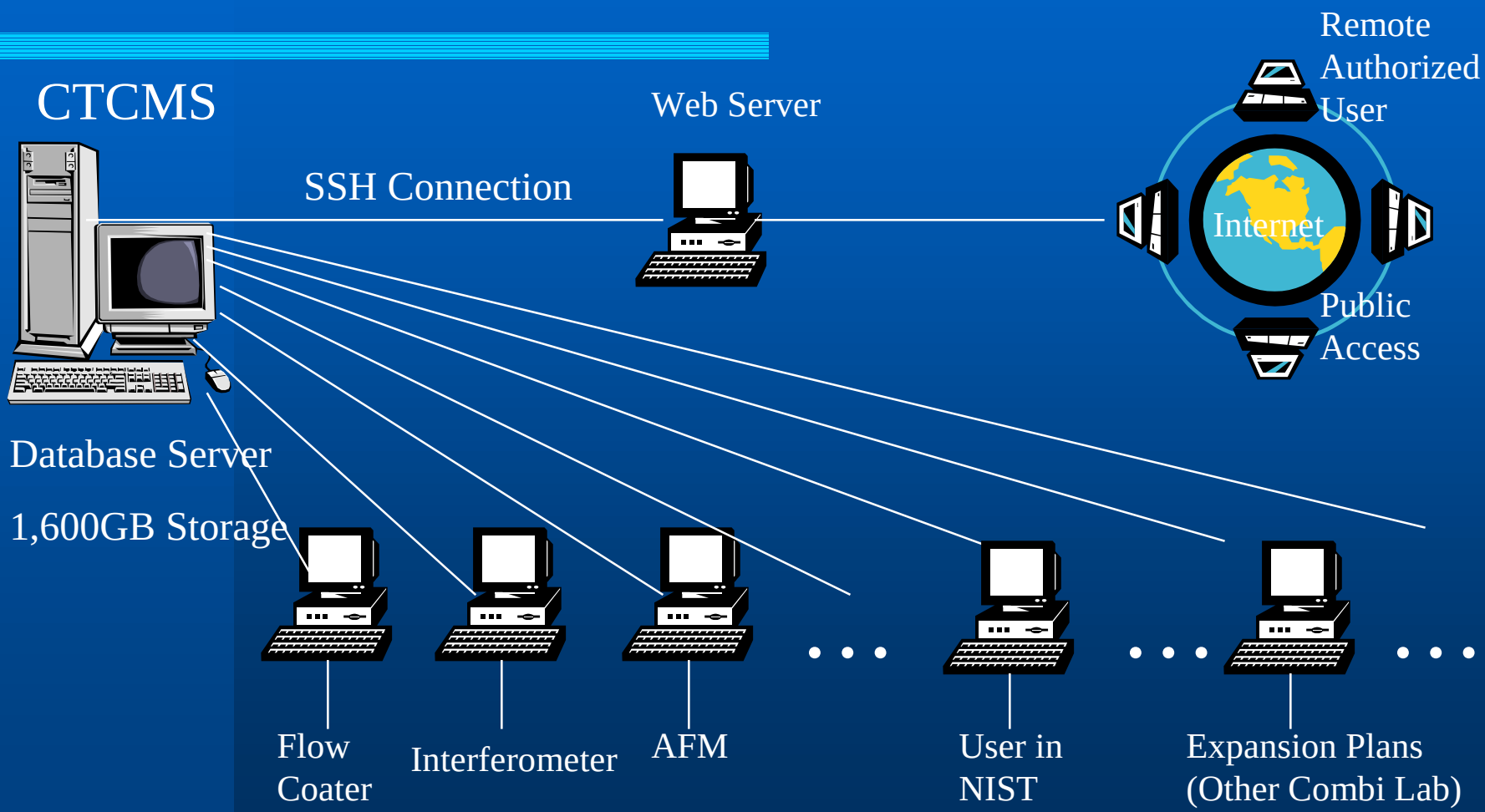
FOR MORE INFO...

WWW.POSTGRESQL.ORG

Software Technology

- **Programming Language**
  - **Python (Open source, Object oriented)**
- **Secured Shell Connection with the Database server**
- **ZOPE selected as Web server**
  - **Base on Python, Open source, Easy to maintain, Database connectivity**
- **Integration with current data analysis software (mostly IDL)**
- **Consideration of future interface with other softwares**

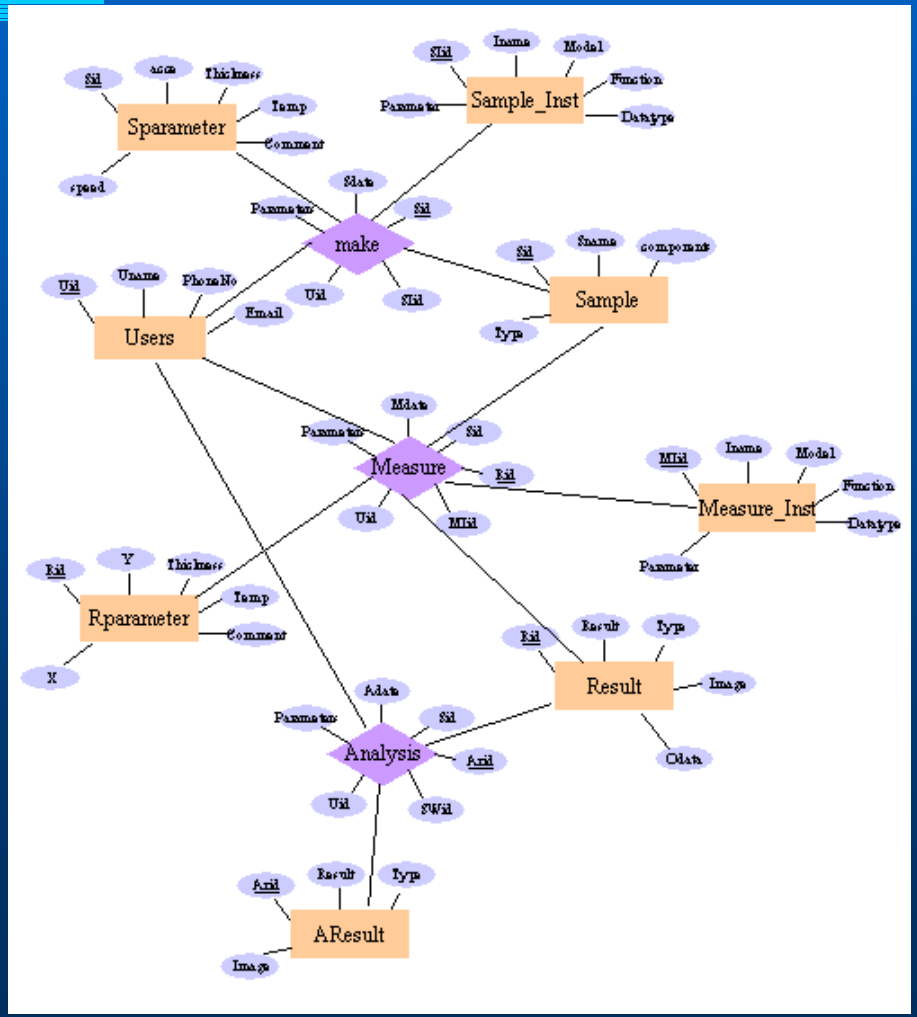
Combi Informatics System

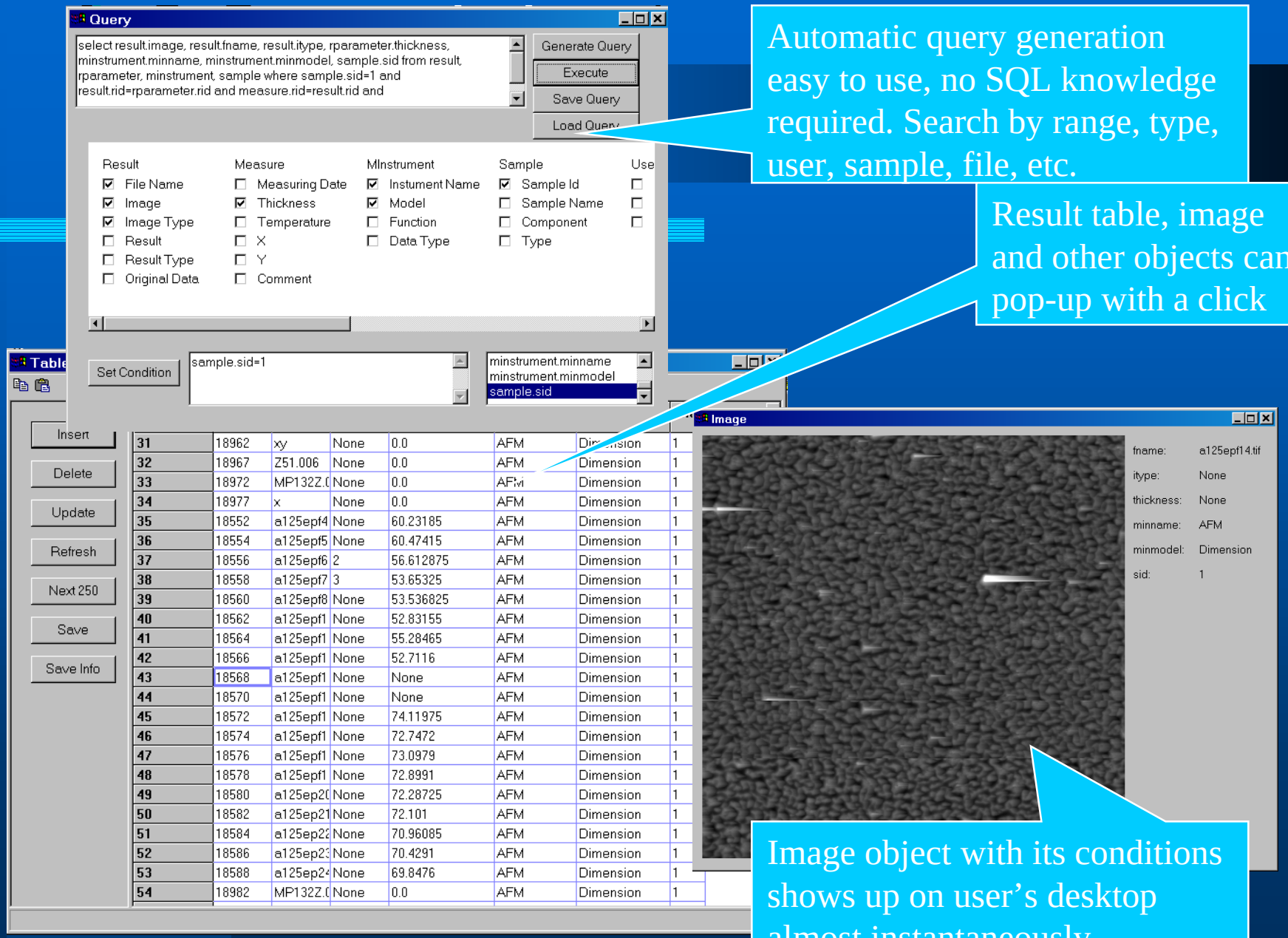


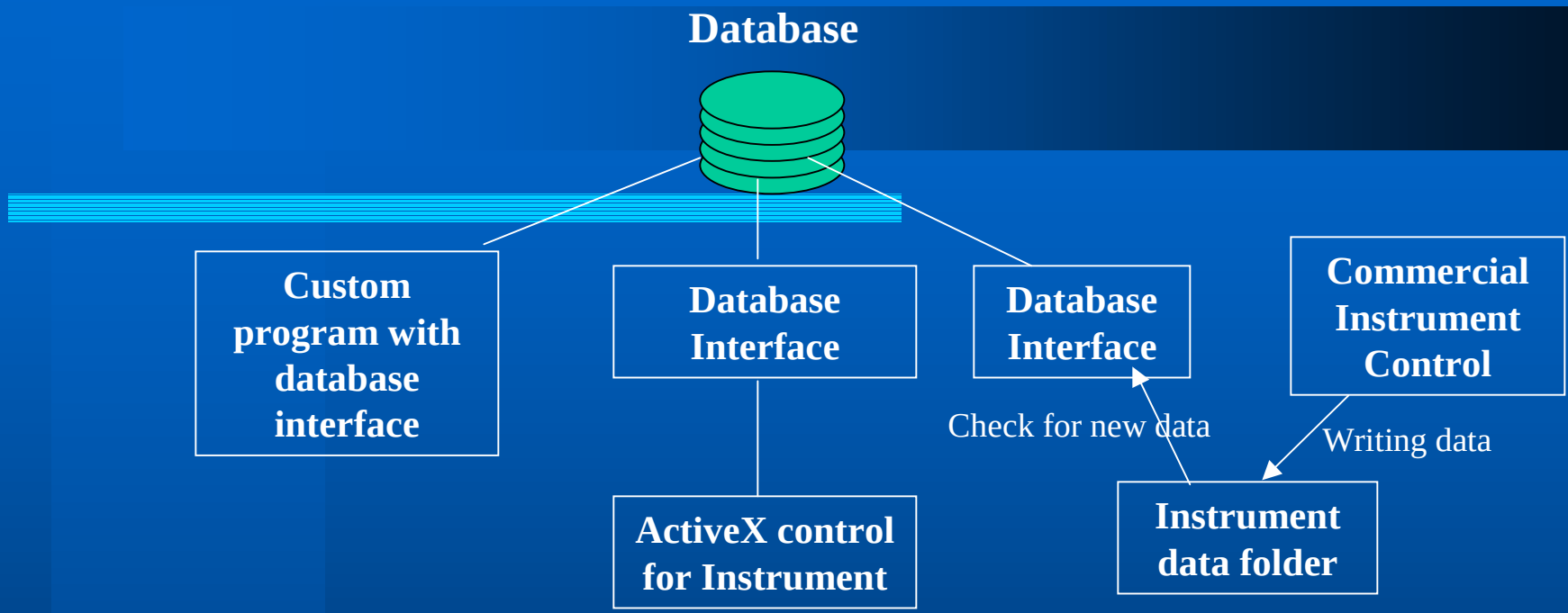
Combi Laboratory Instrument

Basic Structure of Database

- Straight forward structure in consideration of automation & expansion
- Must reflect the frame-work of the Combi lab
- Establish basic protocol of Combi experiment set (All stages of Combi processes)
- Large objects, such as image, video, result chart, original data file storage

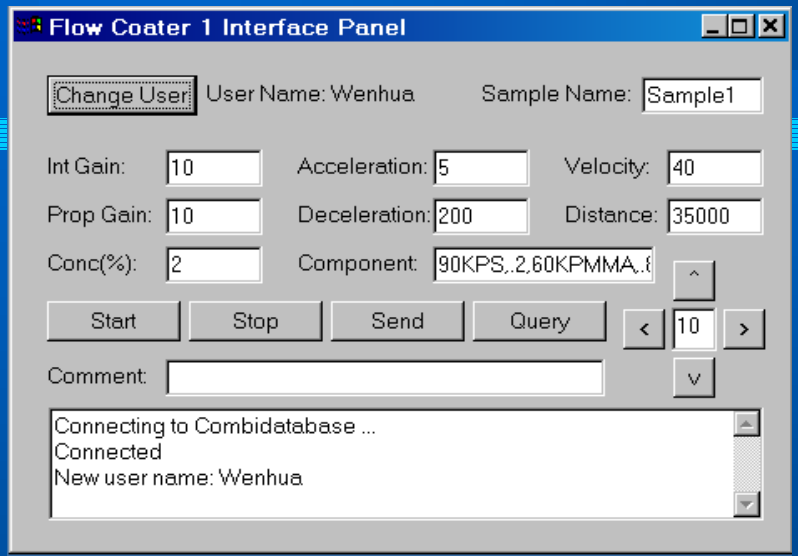


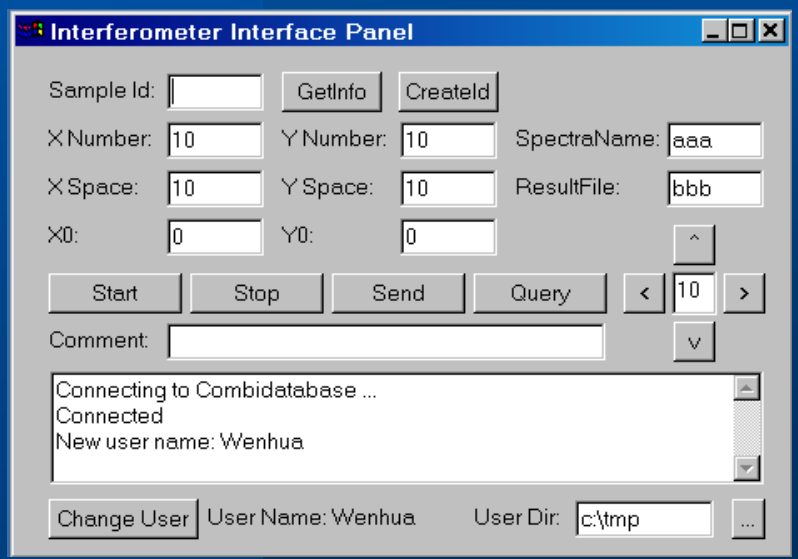

Query
select result.image, result.fname, result.itype, rparameter.thickness, minstrument.minname, minstrument.minmodel, sample.sid from result, rparameter, minstrument, sample where sample.sid=1 and result.rid=rparameter.rid and measure.rid=result.rid and
Generate Query
Execute
Save Query
Load Query
Result
File Name
Image
Image Type
Result
Result Type
Original Data
Measure
Measuring Date
Thickness
Temperature
X
Y
Comment
MInstrument
Instument Name
Model
Function
Data Type
Sample
Sample Id
Sample Name
Component
Type
Use
Set Condition
sample.sid=1
minstrument.minname
minstrument.minmodel
sample.sid
Insert
Delete
Update
Refresh
Next 250
Save
Save Info
31 18962 xy None 0.0 AFM Dimension 1
32 18967 Z51.006 None 0.0 AFM Dimension 1
33 18972 MP132Z.0 None 0.0 AFM Dimension 1
34 18977 x None 0.0 AFM Dimension 1
35 18552 a125epf4 None 60.23185 AFM Dimension 1
36 18554 a125epf5 None 60.47415 AFM Dimension 1
37 18556 a125epf6 2 56.612875 AFM Dimension 1
38 18558 a125epf7 3 53.65325 AFM Dimension 1
39 18560 a125epf8 None 53.536825 AFM Dimension 1
40 18562 a125epf1 None 52.83155 AFM Dimension 1
41 18564 a125epf1 None 55.28465 AFM Dimension 1
42 18566 a125epf1 None 52.7116 AFM Dimension 1
43 18568 a125epf1 None None AFM Dimension 1
44 18570 a125epf1 None None AFM Dimension 1
45 18572 a125epf1 None 74.11975 AFM Dimension 1
46 18574 a125epf1 None 72.7472 AFM Dimension 1
47 18576 a125epf1 None 73.0979 AFM Dimension 1
48 18578 a125epf1 None 72.8991 AFM Dimension 1
49 18580 a125ep20 None 72.28725 AFM Dimension 1
50 18582 a125ep21 None 72.101 AFM Dimension 1
51 18584 a125ep22 None 70.96085 AFM Dimension 1
52 18586 a125ep23 None 70.4291 AFM Dimension 1
53 18588 a125ep24 None 69.8476 AFM Dimension 1
54 18982 MP132Z.0 None 0.0 AFM Dimension 1
Image
fname: a125epf14.tif
itype: None
thickness: None
minname: AFM
minmodel: Dimension
sid: 1
Automatic query generation easy to use, no SQL knowledge required. Search by range, type, user, sample, file, etc.
Result table, image and other objects can pop-up with a click
Image object with its conditions shows up on user's desktop almost instantaneously



Instrument Interface Design Strategy

Custom Progarmming for home made, custom modified instrument

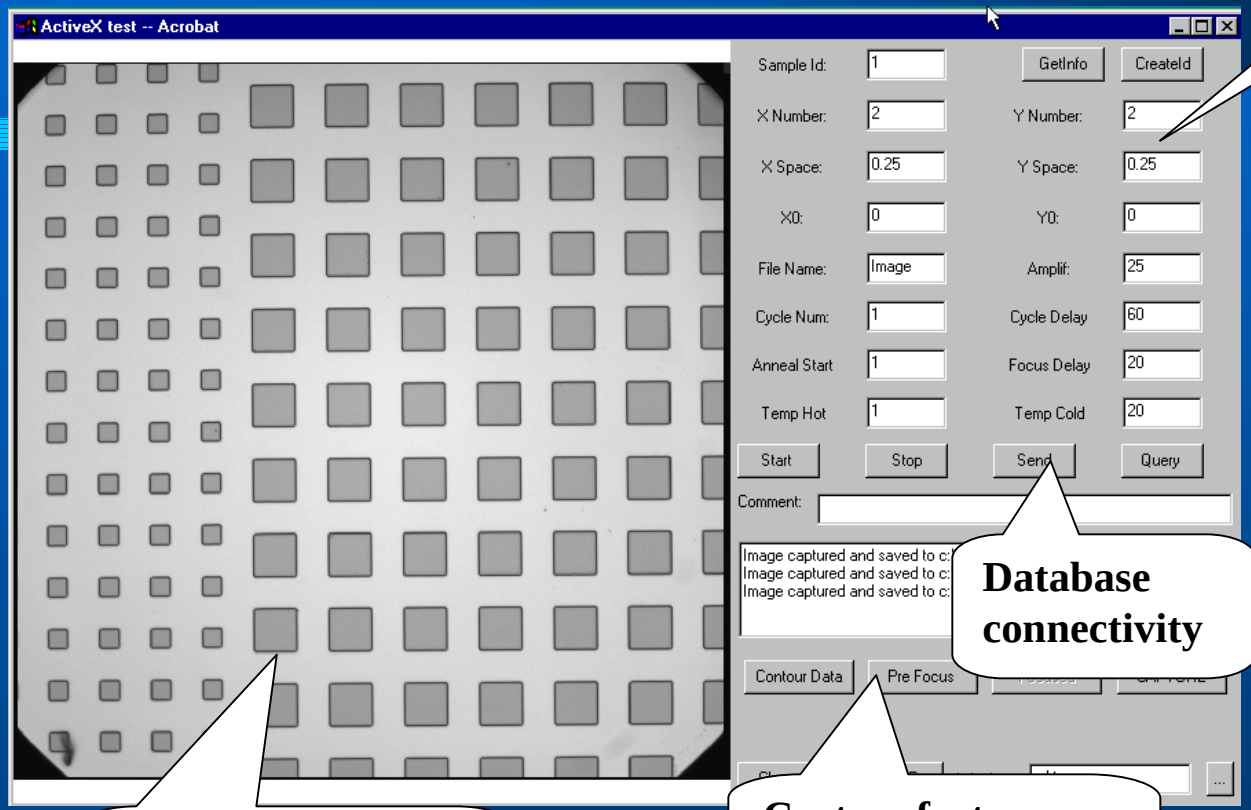




Custom Program for home made instrument that handle both hardware control and Database interface

- **Uniform interface reduce both programming and training time**
- **Parameters are recorded and send to the database automatically**
- **A common query interface that enable inter-instrument communication**
- **Experiment protocol was enforced and data format standardized**
- **Experiment procedure are logged for future reference.**

Using Active-X provided by instrument Vender



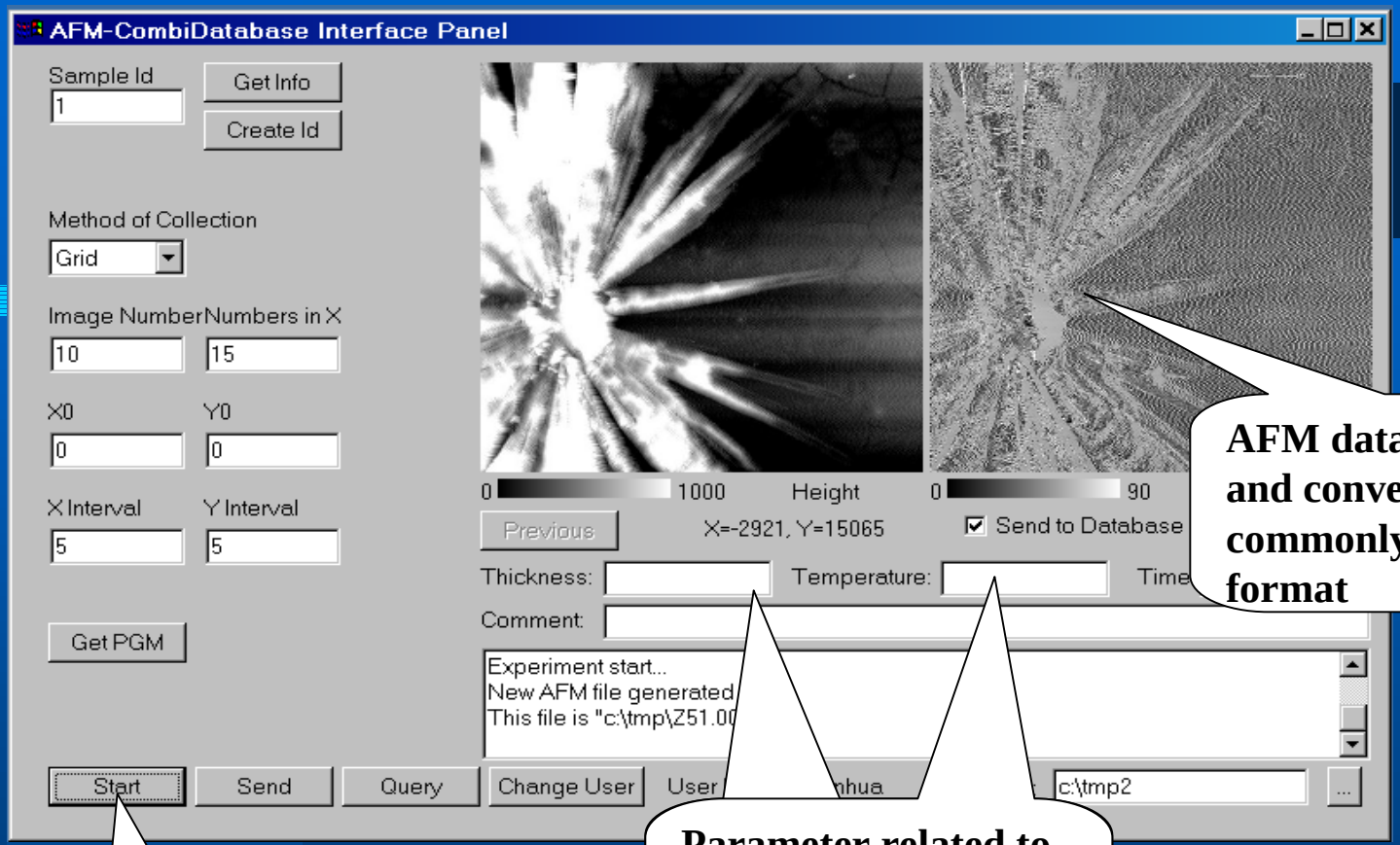
Similer Interface control layout as other instrument.

Database connectivity

ActiveX control provided by vender and control camera to take photos

Custom features are added

- Active X control makes custom instrument control easy to achieve
- add-on features can seamlessly integrated into the program



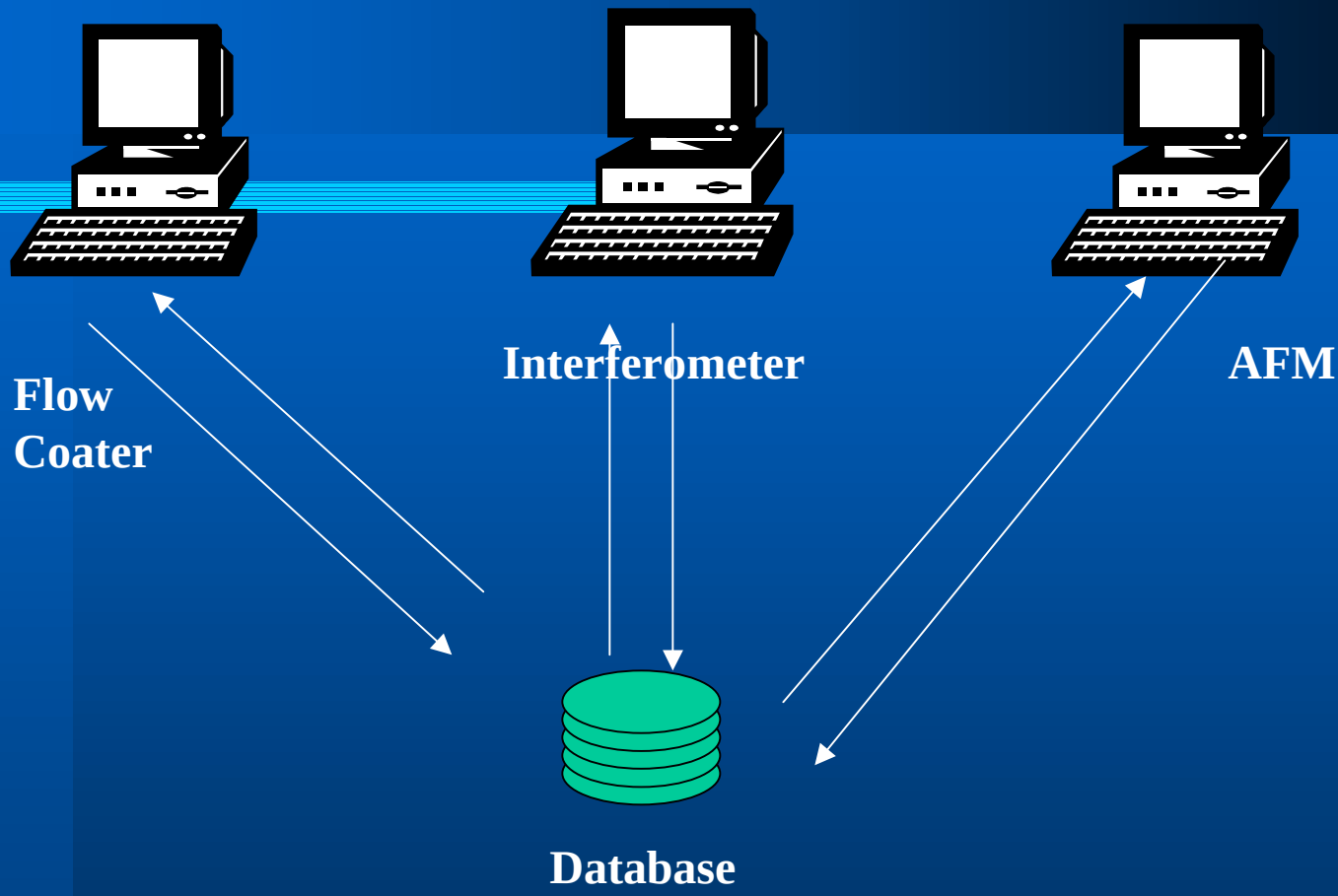
AFM data are parsed and convert to commonly known format

Parameter related to the sample and added on the interface to be send to database

Once experiment start, programming check data folder for new data

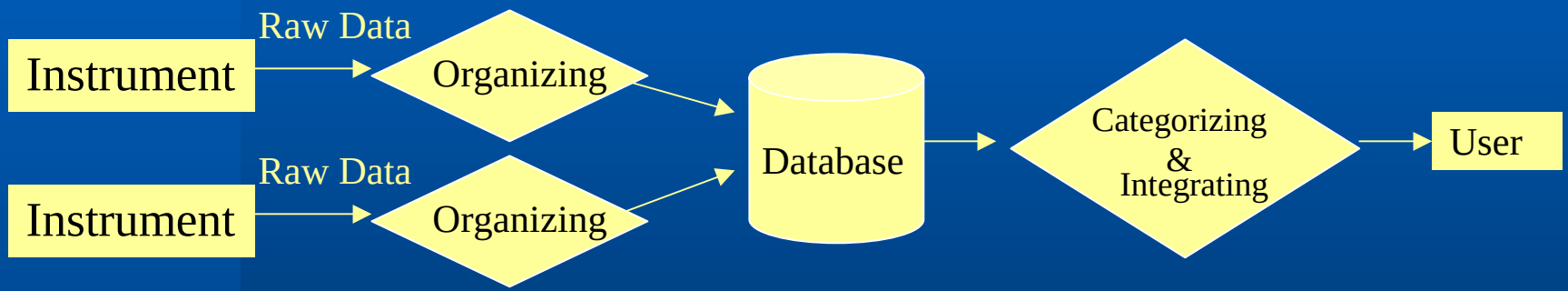
For Instrument without an activeX interface, a backdoor method have to be used to get the data and send it to the database.

Inter-Instrument Communication

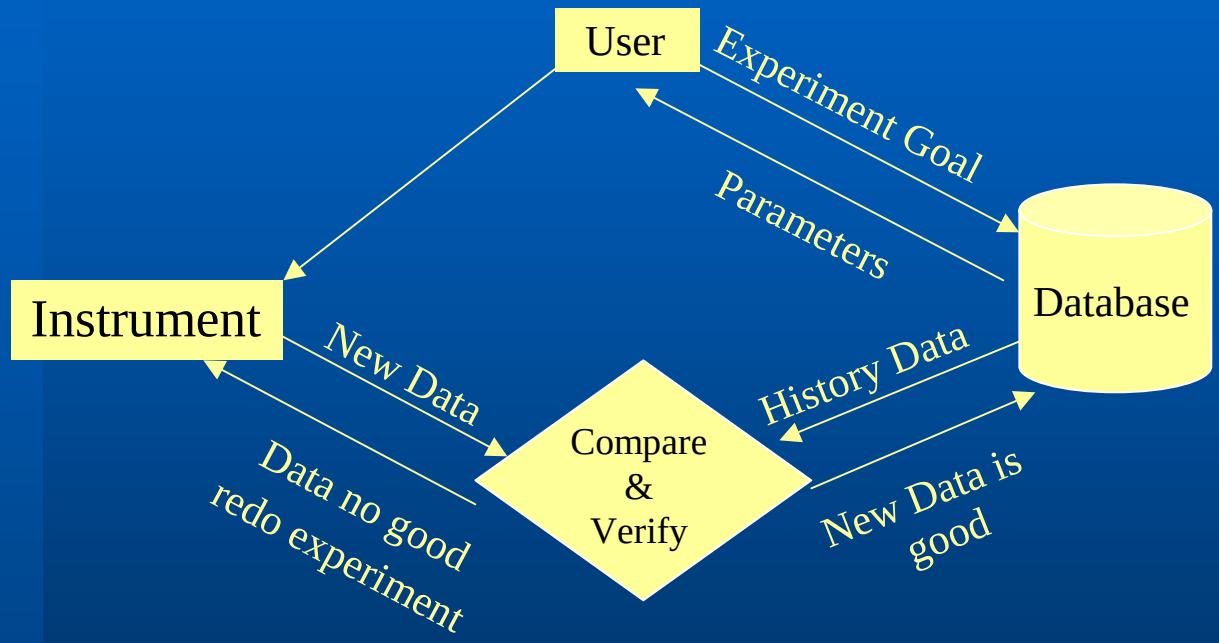


Constantly undated centralized the database make data from one instrument immediately available for other instrument

- Stage1: Automated data entry and retrieval

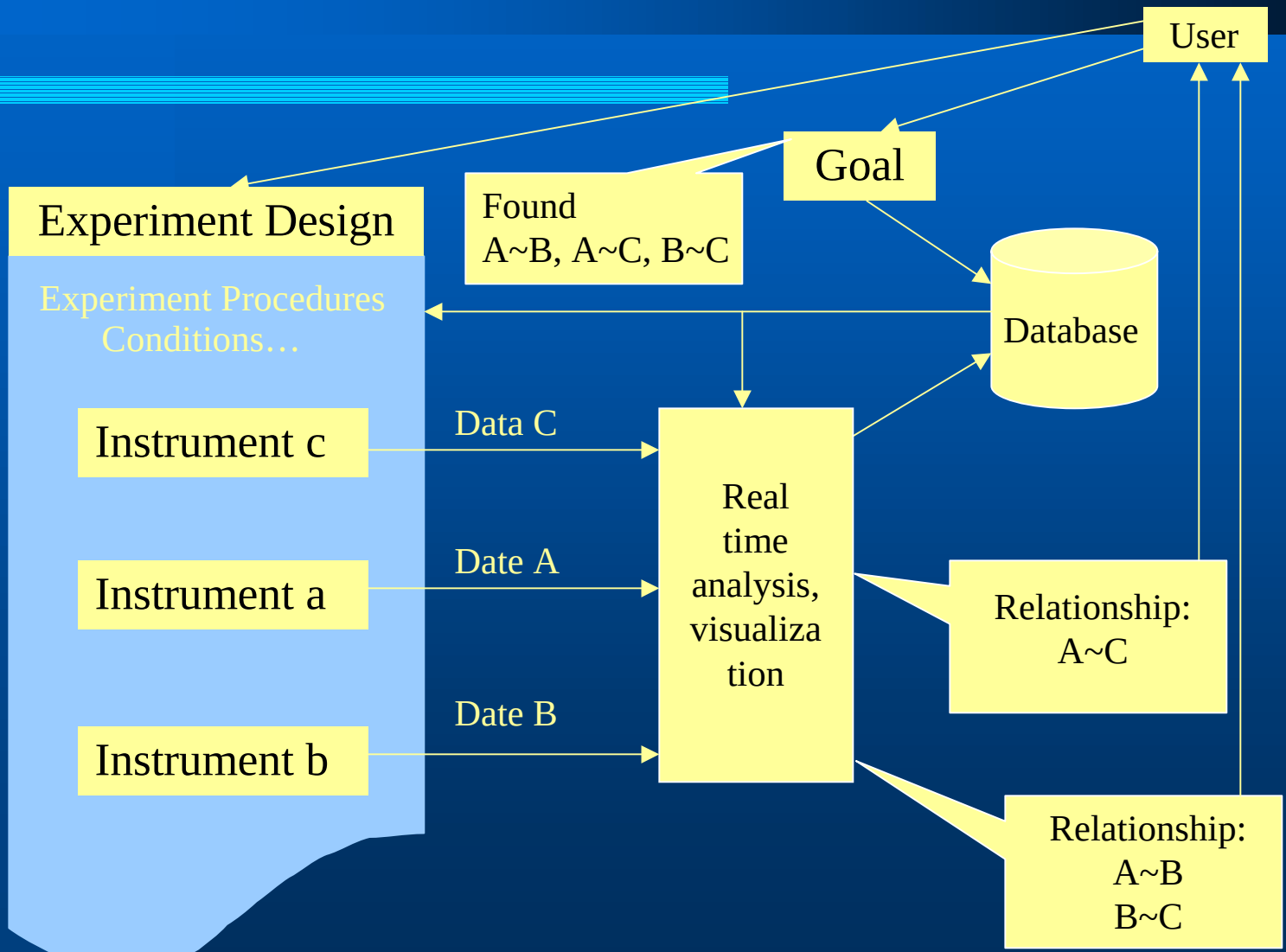


- Stage2: Expert system for each instrument



Online Analysis

- **Stage3:** Closing the loop of the combinatorial method



Challenges:

- How the database will response when the amount of data increases, how to modify the query process to compensate the effect
- Data standard is needed for better inter-instrument communication and easy real time data analysis
- Real time analysis of multi-dimensional data set
- How reliable the automatic data analysis
- How error in data will be handled
- How the database structure will grow when more function are added in the system
- How it interface with other database system

Summary

- The system is designed to streamline and complete a combinatorial workflow geared at accelerated materials research.
- Based on open source code and designed for transparency, we intend this system to be a model for parties interested in building LRIS and a test bed for the development of informatics standards.
- To date, our progress has been in building infrastructure, in particular a centralized database system that includes connections to the instrumentation and analysis tools in our combi facilities.
- We anticipate challenges in developing adequate high-throughput data analysis/datamining software for our system,